SPACE STATION NEUTRAL EXTERNAL ENVIRONMENT

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Abstract. Molecular contamination levels arising from the external induced neutral environment of the Space Station (Phase I configuration) have been calculated using the MOLFLUX model. Predicted molecular column densities and deposition rates generally meet the Space Station contamination requirements. In the doubtful cases of deposition due to material outgassing, proper material selection, generally excluding organic products exposed to the external environment, must be considered to meet contamination requirements. It is important that the Space Station configuration, once defined, is not significantly modified to avoid introducing new unacceptable contamination sources if the contamination requirements are to be met.

Introduction

Deposition of harmful molecular layers on Space Station elements and scientific instruments leading to performance degradation as well as the deterioration of electromagnetic signals from stellar objects due to induced contamination of the environment are a serious concern. They must be assessed as early as possible as part of the Space Station design/development process. The only means to accomplish this is through the use of mathematical models that relate certain Space Station characteristics such as material usage and presence of concentrated gas sources in all locations to their effect on critical instrument/equipment performance. The MOLFLUX program is such a model. If the contamination analysis indicates that a particular Space Station configuration and operating mode leads to "excessive" contamination levels, then design changes must be made (where possible under given circumstances) to reduce this level. On the other hand, once the Space Station configuration is well defined and in all respects acceptable, it should not be significantly modified to avoid introduction of new unacceptable contamination sources. The model predictions discussed in this paper have been produced to provide a preliminary understanding of the effects which the Space Station design may have on meeting its objective. The conclusions reached should play a significant part in the development phase of the Space Station.

Space Station Configuration

The basis for this assessment of the neutral external Space Station environment is the Space Station Phase I configuration. For analysis purposes, the Space Station (solar panels normal to flight direction) is divided into about 300 surface nodes (without the truss) and about 700 nodes including the truss. These as well as a number of "point" nodes represent the potential sources of contamination such as module leakage, gas vents, thrusters, other vehicles (e.g., the Space Shuttle orbiter), outgassing, etc., and receivers of contamination. This system also allows for an assessment of the Space Station interaction with the ambient atmosphere.

Model Description

The MOLFLUX program was developed as an analytical tool to predict the flow

of molecules in the vicinity of vehicles in the space environment. Program output parameters were chosen to address the requirements set by various NASA/contractor contamination working groups including the Space Station External Contamination Working Group (CWG). Program input parameters were selected primarily on the basis that they are fairly easily measurable or at least reasonably predictable. The key to the program itself is a solid scientific foundation. It is based on a numerical integration of the Bhatnagar, Gross, Krook (BGK) model approximation of the Boltzmann kinetic equation for a mixture of gases (Robertson, 1976).

An evaluation of the molecular flow conditions surrounding the Space Station shows that the mean free path of molecules immediately in front of the surface of the large solar panels under ram conditions is on the order of 250 meters. This value, which is based on the assumption of a constant ambient density of approximately 2.1×10^{8} molecules cm^{-3} is large compared with the width of these panels (approximately 10 meters). Therefore a free molecular flow condition exists, with the mean free path increasing rapidly with the distance from the surface. Material outgassing also leads to free molecular flow. At Space Shuttle orbits, where the ambient density is about 10 times as high, the mean free path is about 25 meters, or comparable with the mean orbiter cross section, indicating near free molecular flow conditions. Evaluations such as this one lead to the conclusion that, with few exceptions, either free or "near free" molecular flow exists around spacecraft such as the Space Station in Earth orbit and farther out in space. This conclusion is valid also for thruster plumes with the exception of a small plume volume of viscous and transition flow close to the nozzles or for extremely long firing times.

Accordingly, a model of nearly free molecular flow appears to be adequate to deal with most space-related applications. MOLFLUX has been developed with these thoughts in mind. The distribution function for all species is, therefore, a small perturbation (due to molecular collisions) from the free molecular flow case and allows for backscattering return flux and attenuation calculations. The result is a program of reasonable size and accuracy with maximum flexibility. In general the treatment of data is kept in line with their accuracy, since any model is only as good as the input data used. The capability to introduce input data as well as to evaluate output data is left very general and adaptable to the needs of the user. The model describes the molecular environment in terms of parameters such as local density, column density, direct flux, and return flux (including deposition). The predictions depend on geometric configuration, contamination source characteristics, trajectory/attitude, ambient environment, instrument field-of-view, etc. Predicted direct fluxes involving "points in space," as well as surfaces, are based on line-of-sight (LOS) view factor, distance, and direction calculation techniques. Density and column density are derived from direct flux predictions. One surface reflection (no deposition) was permitted to derive the predicted data in this paper. The model is designed to maximize prediction accuracy specifically in areas where it counts most, i.e., data regarding instrument LOS and instrument field-of-view. The number and location of "space" points are chosen accordingly. Model accuracy is consistent with available input data accuracy as outlined in detail below.

Prediction uncertainties of contamination models are mainly the results of uncertainties of input data.

Part of the molecular deposition on surfaces is caused by backscattering return flux resulting from collisions of contamination molecules with ambient molecules. Elastic molecular collision frequencies and cross sections strongly depend on the velocity distribution of the various molecules involved. Molecular velocities range from thermal velocities all the way up to about 8 km

s^{-1} and more. Present cross section estimates are based on values determined from viscosity measurements since no in situ flight measurements have been performed to date. The MOLFLUX program considers only collisions of high-speed (7.7 km s^{-1}) ambient molecules with local contamination species due to the fact that only these contribute significantly to the backscattered return flux at Space Station altitudes. Under these conditions, the cross section error is estimated to be on the order of a factor 2. Cross section errors of molecules colliding at velocities ranging from thermal to some 10 km s^{-1}, if considered, would be much larger, on the order of a factor 6, increasing the error of return flux predictions accordingly. Since return flux rates are proportional to collision frequencies, the cross section errors translate directly into return flux errors and corresponding deposition rate errors.

Inelastic molecular collisions involving chemical reactions, creation of excited molecules, release of different kind of molecules, etc., do take place, particularly during interaction of ambient high velocity molecules such as atomic oxygen with surfaces (ram cases), modifying the results due to surface reflections and emissions significantly. Unfortunately no quantitative experimental data useful for model inputs are available. Therefore, considerable prediction errors are introduced affecting column density, return flux deposition, and ram cases. Errors due to undefined chemical reactions can amount to some 25%; those due to creation of excited molecules may be significantly larger. The molecular composition of the atmosphere is time- and location- dependent causing an error in return flux and deposition predictions estimated to be about up to a factor of 10 depending on the specific situation.

Surface deposition of molecules is the result of complex processes involving the formation of an equilibrium between impinging molecules and (re-)emitted molecules. This equilibrium is affected by parameters such as surface material and temperature, velocity and kind of impinging molecules, solar radiation, atomic oxygen impact, etc., and therefore, very time dependent. No formula describing adequately the result as a function of all these parameters exists. Accordingly, each case must be analyzed in detail and this has not been done individually for the Space Station. All of the present predictions are the result of very rough estimates based on impinging molecular fluxes. Such predictions may have errors of the order(s) of magnitude(s).

Material outgassing rates depend on material characteristics and the environmental conditions to which the material is exposed including temperature, material history, and exposure history. Such rates have not been adequately formulated to date. Each case must be treated on an individual basis. Current predictions are based on short-term Skylab and Space Shuttle experience generally featuring different materials and may, therefore, vary by orders of magnitude (depending on who is estimating), impacting severely predictions of column densities and molecular deposition rates.

Module leak locations and rates are impossible to adequately define, particularly over long periods of time in thermal and high vacuum environments. Point sources, ring-shaped sources, and area sources have been modeled and basically all lead to very similar results. Presently the Space Station module design leak rate totals 5 lb day^{-1} for practical reasons. There is no proof that the actual leak rate will be smaller or larger than this, particularly over a period of years. An error of a factor 2 may be a reasonable assumption.

Laboratory gas venting is a necessity which can be in conflict with requirements for astronomical observations. The present goal is to design vents and venting procedures which meet both the requirements for adequate venting and astronomy. Preliminary assessments are very encouraging. However, it is too early for a valid error analysis except as discussed in other sections.

The Space Station thruster system design is not well enough defined at this time to permit an acceptable assessment and error analysis. Predictions based on substitute designs may carry significant errors (order of magnitudes).

Since exact solutions to the common gas flow equations such as those named after Boltzmann have not been yet found for general application, analysts are forced to use approximations. Today's prediction techniques, although far from being perfect, however, when applied correctly produce approximation errors which are small compared with the errors introduced by the lack of valid experimental input data.

Predicted Data

Column Density

Module leakage at a total rate of 5 lb day^{-1} has been modeled using several different methods: point sources, ring sources, and area sources. The not so surprising result is that, for any of these, in the worst case, the column density along the module periphery (at about 5 m diameter) is about 3 x 10^{11} for H_2O, 2 x 10^{11} for CO_2, and 1 to 2 x 10^{13} for all gases combined. At reasonable distance of payloads from the modules (leaks), such as 10 m (e.g., locations above the boom) these column densities rapidly drop by a factor 10.

Column densities produced by the whole Space Station (above the contributions from the undisturbed atmosphere) including the effects of module leakage (5 lb day^{-1}), material outgassing (1 x 10^{-11} g cm^{-2} s^{-1}), and ambient gas impingement (ram at ambient of 2 x 10^{8} cm^{-3}) have been calculated for various LOS's originating from a prime measurement point (PMP) located centrally 5 m above the center line of the transverse boom. A typical result (for the LOS in +x direction, direction of flight) is the following: outgassing (M = 100): 0.7 x 10^{10} molecules cm^{-2}, H_2O: 0.2 x 10^{11} molecules cm^{-2}; CO_2: 0.1 x 10^{11} molecules cm^{-2}, and total (all species): 0.6 x 10^{13} molecules cm^{-2}. The docked Space Shuttle adds approximately 25% and the truss itself less than 10% to the total value. The column densities for LOS's in the upper hemisphere are: outgassing: <0.1 x 10^{11}, H_2O: <0.2 x 10^{11}, CO_2: <0.2 x 10^{11}, and total: <0.6 x 10^{13}, all in molecules cm^{-2}, unless the LOS passes near surfaces such as solar panels, payloads, etc.

Column densities of LOS's passing directly in front of solar panels with normals pointing into ram at ambient density of 2 x 10^{8} cm^{-3} are between 1 and 2 x 10^{13} molecules cm^{-2} (induced atmosphere only!).

Column densities produced by small gas vents can be acceptable except for LOS's with points located in the immediate vicinity of the vent(s).

Deposition

Return fluxes due to ambient elastic scattering corresponding to the Space Station column densities defined above for the +x direction and for a field-of-view of 10^{0} (half angle) are as follows: outgassing: 0.5 x 10^{-13}, H_2O: 0.4 x 10^{-14}, CO_2: 0.7 x 10^{-14}, and total: 0.2 x 10^{-11}, all in g cm^{-2} s^{-1}. Return fluxes for LOS's on the wake side of the upper hemisphere have values which are two to three decades lower.

Direct fluxes from the Space Station to a flat surface with its normal in +z direction (vector away from the center of the Earth), at the same PMP, are as follows: outgassing: 0.4 x 10^{-14}, H_2O: 0.8 x 10^{-16}, CO_2: 0.8 x 10^{-16}, and total: 0.1 x 10^{-11}, all in g cm^{-2} s^{-1}. The sources considered here are material outgassing, module leakage and ram condition. These low values are due to the fact that few surfaces are in the field-of-view. Direct fluxes to

the surface with its normal vertical to the +z direction have values in the low 10^{-12} g cm^{-2} s^{-1} range for each of the following species: outgassing, H_2O, CO_2. Direct flux from Space Station surfaces exposed to the ambient atmosphere to a flat plate with its normal in the -x direction (same PMP) totals 0.4×10^{-9} g cm^{-2} s^{-1}.

Actual deposition, based on these rates, depends on surface temperature, surface material, etc. Only a fraction of the outgassing molecules sticks to a surface at ambient temperature.

Molecular deposition on various Space Station elements during Space Shuttle approaches due to thruster firings have been calculated for a great variety of cases involving system engineering simulator (SES) approaches. The results may be summarized as follows: Some of these approaches have produced deposition levels as low as a few Å in thickness on payloads mounted to the transverse boom. The results are very preliminary due to the assumptions made that about 1% of the impinging fluxes remains on the surface and forms a layer of 1 g cm^{-3} density. The deposition levels can be significantly higher if the best available techniques for the Space Shuttle approach are not applied.

Comparison With Requirements

This comparison of predicted data and corresponding requirements is based on the specific assumptions made concerning the values of input parameters and the requirements as defined at this time in JSC 30426. Some of these requirements are briefly summarized below.

Molecular Column Density: For IR active species, such as H_2O, CO_2, etc., 1×10^{11} molecules cm^{-2} each (max. 3×10^{11} total). For non-IR active species, such as O_2, N_2, H_2, noble gases, etc., 1×10^{13} molecules cm^{-2} each (max. 5×10^{13} total).

Molecular Deposition: For 300K surface, 2π sr field-of-view, 1×10^{-14} g cm^{-2} s^{-1}; for 300K surface, 0.1 sr field-of-view, 1×10^{-16} g cm^{-2} s^{-1}; for 5K surface, 0.1 sr field-of-view, 2×10^{-13} g cm^{-2} s^{-1}.

Comparison of molecular column densities indicates that, in all practical situations, the predicted values are well within the requirements. In some extreme cases the predicted values are near the requirement limit. These cases involve rather unrealistic extreme LOS locations/directions such as those directly along "long" surfaces (e.g., near modules and solar panels). In cases where a LOS passes through a local high density gas volume created by leaks or vents, the column density may exceed requirements. However, these cases are easily avoidable.

Comparison of molecular deposition data, assuming "reasonable sticking factors," show that, for the most part, the requirements are met. In the doubtful cases of deposition due to material outgassing resulting from return flux as well as direct surface to surface flux, proper material selection, generally excluding organic products which are exposed to the external environment, is necessary in order to meet contamination requirements. In addition, it appears possible that deposition requirements may be met for the case of Space Shuttle proximity operations, provided that the utmost care is taken to minimize the impingement of contamination fluxes on the Station elements from the Space Shuttle thrusters through optimization of maneuvering procedures.

This data comparison raises concern for possible unacceptable contamination effects, particularly, due to material outgassing. The uncertainty of source

rates and sticking factors as well as of the effects of the layers themselves aggravates this point. The only way to arrive at a fair comparison of predictions and requirements in these questionable cases is to improve the quality of the model input data as discussed later. In addition, it is advisable to compare various model predictions in order to verify significant conclusions and eliminate possible prediction errors.

Affected Space Station Experiments

Certain Space Station experiments may be affected by the induced environment and/or by the interaction with the ambient environment. For instance, measurement of the undisturbed neutral and plasma environment is precluded. Certain measurements may not be possible due to an excessive background. These must be defined through a thorough analysis of sufficient detail and accuracy involving the specific instrument and the predicted environment. The question, "why and to what degree does the particular measurement deteriorate with the presence of a specific amount of a specific species of molecule?" must be clearly answered. At the present time only general categories of measurements may be flagged for potential impacts and further detail study. Operating time of some instruments may be affected by "nonquiescent" periods. Requirements by different types of scientific activity may be in conflict with each other, e.g., venting of gases resulting from processing of materials or stemming from He release by instruments themselves may limit times of astronomical observations and vice versa.

Quantification of Input Data

Presently prediction accuracy limits of contamination models are set by the input data, not the modeling techniques. In order to significantly improve the accuracy of predictions coming from today's contamination flow models, a number of molecular reaction processes and their results must be much better understood. The following are examples of the more important areas:

o Molecular collision frequencies (or cross sections) in the molecular velocity range from thermal to 10 km s^{-1}, particularly near 8 km s^{-1}, must be measured for various specie combinations and excited states. Facilities needed to do this are slowly becoming available.

o Emission and absorption cross sections of molecules must be better known to properly correlate optical effects and molecular column densities. Accommodation coefficients for gases and Space Station surface materials and distribution functions of emitted and reflected molecules must be better defined through measurement.

o Measurement of outgassing rates, particularly long-term, of materials actually used on the Space Station is a necessary goal.

o Knowledge of precise deposition/re-evaporation rates determined in the actual environment (sunlight, atomic oxygen atoms, physical/chemical changes) is mandatory.

o Measurement and definition of processes leading to an accurate understanding of molecular "glow" (ram effect, thruster plumes, etc.) are indispensable.

While all these measurements are necessary, one has to keep in mind, however, that even much improved and highly accurate model predictions are of little value if the actual sensitivity and resulting performance degradation due to the presence of each specific contamination species is not precisely known for comparison. This requires a very active participation of principal investigators (PI's) in the contamination assessment process.

What can be done now? Most, if not all, of these measurements can be performed now, either in the laboratory or on the Space Shuttle.

Conclusion

Molecular column densities and deposition rates predicted by the MOLFLUX model generally meet Space Station contamination requirements. Proper materials, generally excluding organic products exposed to the external environment, must be selected in order to meet contamination deposition requirements. Special sealing considerations must be applied to assure acceptable leakage rates for modules, pressure vessels, fluid containers and associated connections, etc. Molecular deposition due to Space Shuttle proximity operations (thruster firings) can be within requirement limits, provided the maneuvering procedures are optimized.

Reference

Robertson, S. J., Spacecraft Self-Contamination Due to Back-Scattering of Outgas Products, LMSC-HREC TR D496676, Lockheed Missiles and Space Company, Huntsville, Alabama, 1976.